Thermodynamics' 0-th-Law in a nonextensive scenario

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Abstract

Tsallis' thermostatistics [1–14] is by now recognized as a new paradigm for statistical mechanical considerations. However, the generalization of thermodynamics' zero-th law to a nonextensive scenario is plagued by difficulties [2]. In this work we suggest a way to overcome this problem.

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I. INTRODUCTION

Tsallis' thermostatistics offers a suitable and quite significant generalization of the Boltzmann-Gibbs statistical mechanics, that has found multiple applications [1–14]. However, it can not yet comfortably deal with thermodynamics' zero-th law, as pointed out by Tsallis himself in [2]. In [15] Abe has advanced an interesting, tentative solution to the zero-th law conundrum with reference to the micro-canonical analysis of a system composed of two-subsystems in thermal equilibrium. Such an analysis leads to the appearance of temperatures that *depend upon the nonextensive partition function* $\bar{Z}_q$,where q is the Tsallis' non-extensivity index.

As shown by the present authors in a recent study [16], one can recast Tsallis' variational problem (using normalized expectation values) in such a manner that the extremum one thereby finds is guaranteed to correspond to a maximum (and not to other types of extrema) of Tsallis information measure

$$\frac{S_q}{k} = \frac{1 - Tr(\hat{\rho}^q)}{q-1}, \tag{1}$$

($\hat{\rho}$ is the density operator and k is the Boltzmann constant, or more generally, the information unit) because the associated Hessian is diagonal. This treatment involves a new set of Lagrange multipiers λ'_j, to be referred to as the "Optimal set" (OLM), different, but related, to the original Tsallis-Mendes-Plastino (TMP) one (λ_j's) [1]

$$\lambda'_j = \frac{\lambda_j}{\bar{Z}_q^{1-q}}, \tag{2}$$

where the partition function $\bar{Z}_q$ is involved.

Another interesting work in this context is that of Ref. [17], where it is shown that for those particular systems whose partition function is given by $Z_{BG} \propto l^a (\beta')^{-a}$ (a is a dimensionless parameter, and l is a characteristic length), the inverse (thermodynamical) temperature becomes associated with *our* β' and not with the TMP β.

In the present effort we tackle the vexing zero-th law problem starting with the working hypothesis that $1/\beta'$ *is* indeed the temperature. We show that such a hypothesis reconciles

Tsallis' formalism with the zero-th law. A price has to be paid, of course. The important relations [1]

$$\frac{\partial}{\partial E}\left(\frac{S_q}{k}\right) = \beta \tag{3}$$

$$\frac{\partial}{\partial \beta}\left(\ln_q Z_q\right) = -E, \tag{4}$$

lose their basic character, because β depends upon the partition function. They are however recovered in the $q \rightarrow 1$ limit.

We shall tackle the zero-th law problem starting with the hypothesis of [15]: one deals with the Hamiltonian of a system composed of two independent subsystems (in the sense that their mutual interaction is negligible). The system's density operator is product of those pertaining to the subsystems. Before, however, a short recapitulation is necessary.

II. MAIN RESULTS OF THE OLM FORMALISM

The most general quantal treatment is made in a basis-independent way, which requires consideration of the statistical operator (or density operator) $\hat{\rho}$ that maximizes Tsallis' entropy, subject to the foreknowledge of M generalized expectation values (corresponding to M operators $\widehat{O}_j$).

Tsallis' normalized probability distribution [1] is obtained by following the well known MaxEnt route [18]. Instead of effecting the variational treatment of [1], involving Lagrange multipliers λ_j, we pursue the alternative path developed in [16], with Lagrange multipliers λ'_j. One maximizes Tsallis' generalized entropy (1) [10,11,19] subject to the constraints (generalized expectation values) [10,16]

$$Tr(\hat{\rho}) = 1 \tag{5}$$

$$Tr\left[\hat{\rho}^q\left(\widehat{O}_j - \left\langle \widehat{O}_j \right\rangle_q\right)\right] = 0, \tag{6}$$

where $\widehat{O}_j$ $(j = 1, \ldots, M)$ denote the M relevant observables (the observation level [20]), whose generalized expectation values [1]

$$\left\langle \hat{O}_j \right\rangle_q = \frac{Tr(\hat{\rho}^q \hat{O}_j)}{Tr(\hat{\rho}^q)}, \tag{7}$$

are (assumedly) a priori known. The resulting density operator reads [16]

$$\hat{\rho} = \bar{Z}_q^{-1} \left[1 - (1-q) \sum_j^M \lambda'_j \left(\hat{O}_j - \left\langle \hat{O}_j \right\rangle_q \right) \right]^{\frac{1}{1-q}}, \tag{8}$$

where $\bar{Z}_q$ stands for the partition function

$$\bar{Z}_q = Tr \left[1 - (1-q) \sum_j \lambda'_j \left(\hat{O}_j - \left\langle \hat{O}_j \right\rangle_q \right) \right]^{\frac{1}{1-q}}. \tag{9}$$

It is shown in [16] that

$$Tr(\hat{\rho}^q) = \bar{Z}_q^{1-q}, \tag{10}$$

and that Tsallis' entropy can be cast as

$$S_q = k \ln_q \bar{Z}_q, \tag{11}$$

with $\ln_q \bar{Z}_q = (1 - \bar{Z}_q^{1-q})/(q-1)$. These results coincide with those of TMP [1] in their normalized treatment. If, following [1], we define now

$$\ln_q Z_q = \ln_q \bar{Z}_q - \bar{Z}_q^{1-q} \sum_j \lambda'_j \, \left\langle \hat{O}_j \right\rangle_q, \tag{12}$$

we are straightforwardly led to [16]

$$\frac{\partial}{\partial \left\langle \hat{O}_j \right\rangle_q} \left(\frac{S_q}{k} \right) = \bar{Z}_q^{1-q} \lambda'_j \tag{13}$$

$$\frac{\partial}{\partial \lambda'_j} (\ln_q Z_q) = -\bar{Z}_q^{1-q} \left\langle \hat{O}_j \right\rangle_q. \tag{14}$$

Equations (13) and (14) are modified Information Theory relations of the type that one uses to build up, *à la* Jaynes [18], Statistical Mechanics. The basic Legendre-structure relations (of which (3) and (4) are the canonical example) can be recovered in the limit $q \to 1$.

As a special instance of Eqs. (13) and (14) let us discuss the Canonical Ensemble, where they adopt the appearance

$$\frac{\partial}{\partial U_q}\left(\frac{S_q}{k}\right) = \bar{Z}_q^{1-q}\beta' \tag{15}$$

$$\frac{\partial}{\partial \beta'}\left(\ln_q Z_q\right) = -\bar{Z}_q^{1-q} U_q, \tag{16}$$

with (see equation (12))

$$\ln_q Z_q = \ln_q \bar{Z}_q - \beta' U_q. \tag{17}$$

Equations (15) and (16) can be translated into (3) and (4) via (2).

III. THERMODYNAMICAL EQUILIBRIUM

We tackle now the question we wish to address in this effort: to discuss anew the problem of thermodynamical equilibrium on the basis of the results of the preceding Section. Let us consider a composed isolated Hamiltonian system $A + B$, within the framework of the Microcanonical Ensemble. These two subsystems interact via heat exchange.

Following Gibbs, we make the usual assumptions [2]:

1. The interaction energy is negligible

$$\widehat{\mathcal{H}}(A + B) \sim \widehat{\mathcal{H}}(A) + \widehat{\mathcal{H}}(B). \tag{18}$$

2. The subsystems A and B are essentially independent in the sense of the theory of probabilities, i.e.

$$\hat{\rho}(A + B) \sim \hat{\rho}(A)\hat{\rho}(B). \tag{19}$$

The energy distributions are here given, for each system, by specializing (8) and (9) to the instance $M = 1$ and $\hat{O}_1^{(G)} \equiv \widehat{\mathcal{H}}(G),\;\; G = A,\, B$. It easily follows from Eq. (7) that [2]

$$U_q(A + B) = U_q(A) + U_q(B). \tag{20}$$

Now, after a bit of algebra Eq. (1) yields (pseudo-additivity [2])

$$\frac{S_q(A+B)}{k(A+B)} = \frac{S_q(A)}{k(A)} + \frac{S_q(B)}{k(B)} + (1-q)\frac{S_q(A)}{k(A)}\frac{S_q(B)}{k(B)}, \tag{21}$$

which we here recast in the fashion

$$\begin{aligned} &\frac{\ln\left[1+\frac{(1-q)S_q(A+B)}{k(A+B)}\right]}{1-q} = \\ &= \frac{\ln\left[1+\frac{(1-q)S_q(A)}{k(A)}\right]}{1-q} + \frac{\ln\left[1+\frac{(1-q)S_q(B)}{k(B)}\right]}{1-q}, \end{aligned} \tag{22}$$

where we have made it explicit the fact that the constant k could, eventually, depend upon the system's nature.

Focus attention now upon Eqs. (20) and (22). For a closed system, both energy and entropy are conserved. As a consequence:

$$\delta U_q(A) = -\delta U_q(B), \tag{23}$$

$$\frac{1}{Tr[\rho(A)]^q}\delta\left(\frac{S_q(A)}{k(A)}\right) = -\frac{1}{Tr[\rho(B)]^q}\delta\left(\frac{S_q(B)}{k(B)}\right). \tag{24}$$

Introduction of (10) into (24) yields now

$$\frac{1}{\bar{Z}_q(A)^{1-q}}\delta\left(\frac{S_q(A)}{k(A)}\right) = -\frac{1}{\bar{Z}_q(B)^{1-q}}\delta\left(\frac{S_q(B)}{k(B)}\right). \tag{25}$$

The next step is to consider the ratio between (25) and (23), keeping in mind (15). One immediately finds the equality

$$\beta'(A) = \beta'(B), \tag{26}$$

i.e., if we set $\beta' \propto 1/T$, thermal equilibrium between A and B arises in a natural fashion and the *thermodynamics' zero-th law* is obtained. This constitutes the essential result of the present effort. Notice that one assumes here that β', not β (as in [15]), is proportional to $\frac{1}{T}$, a fact first observed in [17] for those special systems whose partition function is of the form $Z_{BG} \propto l^a(\beta')^{-a}$, with a a dimensionless parameter, and l a characteristic length.

In terms of β (the TMP Lagrange multiplier) we have

$$\frac{\beta(A)}{\bar{Z}_q^{1-q}(A)} = \frac{\beta(B)}{\bar{Z}_q^{1-q}(B)}. \tag{27}$$

To take β as proportional to $\frac{1}{T}$ forces one to work with a temperature that depends upon the partition function [15].

The present work shows that one can reconcile the zero-th law with Tsallis' thermostatistics without going to the limit $q \to 1$. In order to assess to what an extent have we succeeded it remains to ascertain the self-consistency of the Gibbs' hypothesis (18,19) within our nonextensive framework. We reconsider the application of Eq. (8) to our present situation and define

$$\widehat{F}(A) = \left[1 - (1-q)\beta\left(\widehat{\mathcal{H}}(A) - U_q(A)\right)\right]^{\frac{1}{1-q}}, \tag{28}$$

with a similar expression for $\widehat{F}(B)$. We have then

$$\hat{\rho}(A)\hat{\rho}(B) = \frac{\widehat{F}(A)}{\bar{Z}_q(A)}\,\frac{\widehat{F}(B)}{\bar{Z}_q(B)}, \tag{29}$$

which, after explicit evaluation, and keeping just first order terms gives

$$\begin{aligned}\hat{\rho}(A+B) &= \hat{\rho}(A)\hat{\rho}(B) - \\ &-(1-q)\beta^2\frac{[\widehat{\mathcal{H}}(A) - U_q(A)]}{\bar{Z}_q(A)}\frac{[\widehat{\mathcal{H}}(B) - U_q(B)]}{\bar{Z}_q(B)},\end{aligned} \tag{30}$$

which is the promised result. As pointed out in [22], our subsystems are not exactly independent. But the last term on the r.h.s. of the above expression is negligible for i) high temperatures, ii) the thermodynamic limit (see below), or, of course, for iii) q-values close to unity.

IV. CONCLUSIONS

We have carefully reconsidered the validity of the zero-th law of thermodynamics in a Tsallis' environment. It has been shown to remain approximately valid.

The question revolves around the independence of two independent subsystems and A, B that are brought into thermal contact. We have found that they can indeed be regarded as independent in quite important instances:

- 1) $q \to 1$, of course,
- 2) in the high temperature limit, and
- 3) *for systems in contact with a heat reservoir*, because, if A, say, is the reservoir, $[\widehat{\mathcal{H}}(A) - U_q(A)]$ is a null operator (the mean energy of a reservoir coincides, by definition, with one of its eigenenergies [24]). Now you invoke implicitly the heat reservoir notion whenever you use a thermometer!

Summing up, for practical purposes the zero-th law of thermodynamics is valid in a Tsallis scenario.

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